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Update to “Computational Aspects of Nitrogen-Rich HEDMs”

by Betsy M Rice, Edward FC Byrd, and William D Mattson

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Weapons and Materials Research Directorate, ARL

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14. ABSTRACT <p>Further computational studies and improved methods leading to prediction of properties and behavior of high-nitrogen materials continue as both computational capabilities and methods advance. As detailed in the 2007 book chapter titled “Computational Aspects of Nitrogen-Rich HEDMs” [Rice BM, Byrd EFC, Mattson WD. Struct Bond. 2007;125:153–194], a multitude of models were developed to predict key performance properties of energetic materials that include numerous high-nitrogen systems based on atomistic quantum mechanical simulations. In this report we will provide updates to these developments. Additionally, a number of theoretical studies have since been undertaken to explore the structure and behavior of novel condensed phases of polymeric nitrogen. This work shall outline advances in the field since its first publication in 2007.</p>					
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1. Introduction

A high-energy-density material (HEDM) must meet multiple various performance and material properties before selection for inclusion in a munition. These properties range from critical performance properties, such as heats of formation and crystalline densities (key for determining detonation and propellant performance), to melting points, compatibility with other formulation materials, sensitivities to insult, and environmental impact. While most research has focused on heats of formation and densities, researchers have begun investigating whether models can be developed for the prediction of other properties. In this report, we will present successes and failures for several properties.

2. Crystal Densities

Beginning with crystalline densities, there have been numerous approaches to predict the density without any experimental knowledge of the system under study. These methods can be broken into 2 main camps: those based on building full 3-dimensional (3-D) representations of the crystal (ab initio crystal prediction) and those based on models using only the information obtained from a single isolated molecule (molecular volumes). Both of these methods have been summarized in Rice et al.¹ and both have demonstrated some success.

While ab initio crystal prediction methods can provide both predicted densities and X-ray spectra, these methods are usually computationally intensive and/or typically require the use of classical force fields, which must be constructed and/or tested for the molecular system of interest. For a more recent series of review articles on crystal structure prediction methods, see Atahan-Evrenk and Aspuru-Guzik.² As only the density is required for use in predicting performance properties, we shall focus on methods yielding solely the density. In our earlier work,³ we initially correlated the crystal density to a simple functional:

$$\rho = \frac{M}{V_M}, \quad (1)$$

where M was the molecular mass of the single molecule and V_M was the volume inside the 0.001 au isosurface of electron density surrounding the molecule, which was calculated using the B3LYP/ 6-31G**⁴⁻⁶ density functional theory (DFT) as implemented in the Gaussian program package.⁷ Applying this method to 180 neutral carbon-hydrogen-nitrogen-oxygen (CHNO)-containing molecules and 38 high-nitrogen systems yielded root-mean-square (rms) percent deviations of 3.7% and 3.4%, respectively, compared to experiment. When applied to ionic molecules, the resultant predictions were worse, with a 6.6% rms disagreement from

experiment. While applying a correction based on the number of hydrogens in the moiety improved the results somewhat (4.8% rms error), later refinements to the model, founded on the works of Politzer et al.^{8,9} suggesting the addition of corrections based on electrostatic interactions, would provide an improved correlation. In reparametrizing equations from the Politzer et al. approach, we significantly improved the crystal density predictor with new rms errors of 2.7% for neutral molecules (on 38 test molecules) and 3.7% for ionic systems (on 48 test molecules).¹⁰ Equations 2 and 3 were used for the neutral and ionic density predictors.

$$\rho = \alpha_1 \left(\frac{M}{V_M} \right) + \beta_1 (v \sigma_{tot}^2) + \gamma_1. \quad (2)$$

$$\rho = \alpha \frac{M}{V_M} + \beta \sum \left(\frac{\overline{V_S^+}}{A_S^+} \right) + \gamma \sum \left(\frac{\overline{V_S^-}}{A_S^-} \right) + \delta. \quad (3)$$

For the neutral molecule equation, σ_{tot}^2 is the total variance of the electrostatic potential mapped onto the 0.001 au isosurface of electron density of the isolated molecule; v quantifies the degree of balance between the positive and negative potentials on the molecular surface. For the ionic molecule equation, $\overline{V_S^+}$ is the average of the positive values of the electrostatic potential on the 0.001 au molecular surface V_S , and A_S^+ is the portion of the cation's surface that has a positive electrostatic potential. Likewise, $\overline{V_S^-}$ is the average of the negative values of V_S , and A_S^- is the portion of the anion's surface that has a negative electrostatic potential. These ratios are summed for each charge moiety in the total ionic system. The terms α_1 , β_1 , γ_1 , α , β , γ , and δ are all fitted constants.

3. Solid Phase Heats of Formation

The second of the 2 key performance properties, the solid phase heat of formation, traditionally has been a computational challenge. While there exist numerous methods of varying accuracy and computation cost for predicting the gas phase heats of formation, the lack of an adequate treatment of the cohesive forces binding the disparate molecules together into a solid has hampered the prediction of this property. The methods existent to date have relied mostly on fitted quantitative structure property relationships (QSPRs), correlating electronic structure properties to experimental data. In Rice et al.¹, we illustrated a QSPR method for neutral molecules that displayed reasonable accuracy. However, we demonstrated there were no accurate predictive tools for ionic compounds. In 2009, Byrd and Rice¹¹ examined a host of different methods to compute the gas phase heats of formation along with different models to determine the lattice enthalpy, which, when added, will produce the desired solid phase heat of formation. Two methods were used to

compute the gas phase heats of formation, the very accurate (and computationally expensive) G3MP2B3 theory^{12,13} and a more empirical scheme, while 6 methods were used to determine the lattice enthalpies. These methods ranged from extended lattice summations (requiring the crystal structure, a necessary property obtained through computationally costly crystal structure prediction calculations for notional compounds) to QSPR methods.

The most recognized QSPR model to calculate lattice enthalpies used was designed by Jenkins et al.¹⁴⁻¹⁶ and was fitted to large molecular anions but composed mostly of small alkali metal and alkaline earth cations (Li, Na, K, Rb, Cs, Mg, Ca, Sr, Ba). This restricted parameterization is of concern when applied to ionic high-nitrogen materials, as most of the anions are not monoatomic species. Fortunately, there exists a reparametrized version of the Jenkins method for the 1:1 salts, developed by Gutowski et al.,¹⁷ that uses the same functional form but corrects this deficiency in the original fitting set. Both of these models have an inverse cube root dependence on the formula unit volume, which can be computed as described above.

The method determined to yield the most accurate results for the condensed phase heat of formation was the combination of G3MP2B3 theory (gas phase heat of formation) with the Gutowski method of calculating the lattice energy (24 kcal/mol rms error), but this method is restricted to 1:1 salts. For all other salts, the G3MP2B3 theory with the Jenkins method provided results that were within 5 kcal/mol rms error of the more accurate lattice summation methods (36.6 kcal/mol vs. 31.2 kcal/mol rms errors). This is fortunate, as the Jenkins and Gutowski models require no experimental information, can be rapidly obtained with very modest computational resources, and produce results that are approximately as accurate as those obtained using more computationally costly methods that explicitly calculate interatomic interactions in an ionic crystal.

Byrd and Rice¹¹ also showed the effect on predicted lattice enthalpies using formula unit volumes based on the refined densities using electrostatic potential information. Using the updated crystal density predictors, and then converting these to formula unit volumes (by dividing the formula unit mass by the updated predicted density), we observed minimal change in the predicted lattice enthalpies, on the order of 1.4 kcal/mol average absolute difference.⁹ This was expected; overall, the volume changes were minor, and once filtered through an inverse cube root (the functional form of the Jenkins method), the resultant differences were minute.

4. Prediction of Vulnerability, Hazard, and Other Properties

While there has been significant focus on the prediction of performance properties of high-nitrogen materials, these are not the only factors to consider when pursuing novel energetic materials. Other concerns of note are sensitivity to insult (e.g., impact, friction, electrostatic discharge), physical properties (e.g., melting points), environmental impact, and toxicity as well as compatibility with formulation ingredients. These additional properties, however, usually involve complex, dynamic processes that do not lend themselves well to “simple” predictive techniques as illustrated previously. A prime example of this is the prediction of impact sensitivity of energetic materials. There exists scores of proposed methods to predict impact sensitivities through the correlation of molecular or material properties, yet to date, none has demonstrated stellar success. Our own efforts in this field have ranged from semi-empirical QSPR-based methods (8 descriptor multivariate linear regression equations yielding an R^2 of 0.75)¹⁸ to attempted correlations of electrostatic properties on the partitioned quantum mechanical electron density derived from Bader’s atoms-in-molecules technique.^{19,20} For these studies, while many correlations were attempted, and several approximate correlations were determined, all exhibited limited predictive capability, and no accurate quantitative correlations were found. To date, there exists no accurate, universal predictive methodology for sensitivities for energetic materials.

Another property that has garnished considerable attention is the prediction of the melting point of a material. The most common approach used is that for QSPRs, which have demonstrated some successes for this challenging problem, some of which were developed for conventional energetic materials.²¹ In a recent paper,²² Morrill and Byrd use the AM1 semi-empirical quantum mechanical method to design multivariate linear relationships based on the experimental melting points for over 100 high-nitrogen compounds. The models resulting from this study had R^2 values of 0.94 and 0.90 on the test sets for the 2 QSPRs developed (rms errors of ± 7.0 and ± 8.8 °C, respectively), which rank among the best melting point models published for energetic materials.

5. Novel Polynitrogen Species and Novel High-Pressure Phases of Nitrogen

The relatively modest computational resources required to obtain basic molecular information using DFT have resulted in a proliferation of computational studies of isolated high-nitrogen molecules and will not be reviewed here. However, the advances in high-performance computing, scalable DFT codes, and crystal

structure prediction algorithms have allowed theoretical explorations of structure and behavior of novel high-pressure phases of polymeric nitrogen since “Computational Aspects of Nitrogen-Rich HEDMs”¹ was published. One of us performed quantum-based molecular dynamic (QMD) simulations in which a shock wave was initiated into a long 3-D filament of cubic gauche nitrogen (cg-N)²³ through flyer plate impact. The shock response of the filament was quite different from that which we observed in QMD simulations of the shocked conventional energetic material pentaerythritol tetranitrate (PETN). In PETN, we observed heat release reactions directly behind the shock front, while in the shocked cg-N simulations, a series of energy-absorbing phase transformations and spontaneous defect formations occurred immediately behind the shock front. The decomposition of the polymeric matrix occurred at the far edge of the filament opposite to the traveling shock front; the heat generated in this decomposition did not contribute to driving the front.

A follow-up effort by Beaudet and Mattson²⁴ focused on attempts to generate ambient pressure amorphous polymeric nitrogen condensed phases, known to exist at low temperatures up to 100 K.²⁵ Generation of amorphous structures using standard simulated annealing methodologies and DFT was challenging, leading us to initiate the structure search using semi-amorphous parts of the highly defected shock region in the cg-N simulation. Thermal annealing and optimization led to the discovery of a novel low-pressure porous crystalline form of nitrogen. The study was also particularly useful in identifying defects as sources of instability in the crystal, information that could be used to guide stabilization efforts. Other unusual structures of pure all-nitrogen crystals have been theoretically explored, including a molecular crystal of N₈ molecules, whose main crystal forces are weak van der Waals and electrostatics; this crystal is predicted to be metastable at ambient pressure.²⁶ Crystal structure predictions of all nitrogen systems at terapascal (TPa) pressures produced several stable phases, with one surprising metallic phase consisting of N₅ and N₂ moieties and exhibiting ionic features and charge density distortions.²⁷ Another group performed a crystal structure prediction search that produced an N₁₀ cage-like diamonoid structure stable at pressures above 260 gigapascals (GPa).²⁸

Heteroatomic mixtures of polymeric nitrogen have also been explored to increase stability and otherwise optimize material properties. Polymeric nitrogen forms are found for compressed systems of various hydrogen-nitrogen mixtures,^{29–31} sodium azide,^{32,33} CO with N₂,^{34,35} and N₂O³⁶. Polymeric nitrogen has also been encapsulated within nanotubes, both carbon³⁷ and silicon carbide.³⁸ Finally nanotube crystals of nitrogen-nitrogen-oxygen (NNO) and nitrogen-phosphorous-oxygen (NPO) were found through crystal structure prediction methods.³⁹ While

the NNO extended solid is not stable at ambient pressure, the NPO crystal was found to be stable at zero pressure and has an energy content 86% higher than 1,3,5,7-tetranitro-1,3,5,7-tetra-azacyclo-octane (HMX).

6. Conclusions

Increased interest in developing these novel high-nitrogen materials, particularly the novel high-pressure condensed phases of polymeric forms of nitrogen, will continue to benefit from theoretical predictions of structure and properties of the materials, particularly in providing guidance in design and stabilization.

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List of Symbols, Abbreviations, and Acronyms

6-31G**	Pople's Gaussian double-zeta polarized basis set with d polarization functions on each of the atoms Li through Ca and p polarization functions on H and He
v	balance parameter
Σ	average electrostatic surface potential
σ^2	variance of electrostatic surface potential
ρ	crystalline density
AM1	semi-empirical method
APG	Aberdeen Proving Ground
ARL	US Army Research Laboratory
au	atomic unit
Ba	barium
B3LYP	Becke 3 parameter exchange with Lee-Yang-Parr correlation DFT functional
Ca	calcium
cg-N	cubic gauche nitrogen
CHNO	carbon-hydrogen-nitrogen-oxygen
Cs	cesium
DFT	density functional theory
G3MP2B3	G3 variant that uses MP2 instead of MP4 for the basis set extension corrections and uses the B3LYP structures and frequencies instead of the Hartree-Fock values
GPa	gigapascal
HEDM	high-energy-density material
HMX	1,3,5,7-tetranitro-1,3,5,7-tetra-azacyclo-octane
K	potassium
kcal/mol	kilocalories per mole (unit of energy)

Li	lithium
M	molecular mass
Mg	magnesium
Na	sodium
NNO	nitrogen-nitrogen-oxygen
NPO	nitrogen-phosphorous-oxygen
PETN	pentaerythritol tetranitrate
QMD	quantum-based molecular dynamics
QSPR	quantitative structure property relationships
R ²	coefficient of determination
Rb	rubidium
Sr	strontium
TPa	terapascal
rms	root mean square
V	electrostatic potential
V _M	volume inside the 0.001 au isosurface of electron density surrounding the molecule

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